

# Effective Hamiltonians for fastly driven tight-binding chains

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We consider a single particle tunnelling in a tight-binding model with nearest-neighbour couplings, in the presence of a periodic high-frequency force. An effective Hamiltonian for the particle is derived using an averaging method resembling classical canonical perturbation theory. Three cases are considered: uniform lattice with periodic and open boundary conditions, and lattice with a parabolic potential. We find that in the latter case, interplay of the potential and driving leads to appearance of the effective next-nearest neighbour couplings. In the uniform case with periodic boundary conditions the second- and third-order corrections to the averaged Hamiltonian are completely absent, while in the case with open boundary conditions they have a very simple form, found before in some particular cases by S.Longhi [Phys. Rev. B 77, 195326 (2008)]. These general results may find applications in designing effective Hamiltonian models in experiments with ultracold atoms in optical lattices, e.g. for simulating solid-state phenomena.

## I. INTRODUCTION

Effective Hamiltonians created by high-frequency perturbations have many interesting applications in physics; a well-known counterintuitive example of induced effective potential is provided by Kapitza pendulum [1, 2]. We are interested in applying averaging methods of classical Hamiltonian mechanics (see, e.g., [3]) to quantum tight-binding models, which often arise in solid-state and, more generally, condensed-matter physics.

In solid-state physics, unusual transport phenomena may arise when an ac electric field is applied to the system, e.g. coherent destruction of tunnelling and dynamic localization [4, 5]. Corresponding applications to coherent control of tunnelling and electronic transport in semiconductor superlattices and arrays of coupled quantum dots have been receiving a lot of interest lately [6, 7]. Very recently, in many experiments with atoms in optical lattices, effective Hamiltonians were created using high-frequency perturbations [5, 8, 9]. A particle in a deep optical lattice potential can be described by a tight-binding model. Applying a high-frequency force, one can engineer effective tunnelling constants in the model, which can be useful to mimic certain solid-state phe-

nomena [8]. For many realistic applications of such type, it is important to derive accurate effective Hamiltonians taking into account higher-order terms [10]. Here we find a useful method for such derivation in the spirit of canonical perturbation theory, and apply it for several tight-binding systems. Our approach is based on idea of canonical transformations removing time-dependence from the Hamiltonian, which in the present context means unitary transformations of square matrices. Similar ideas have been applied to transport in classical periodic potentials [11–13]. In the next Section, the general method is outlined. In Section III, it is applied to three different tight-binding models. Our approach is actually not limited to tight-binding systems, but it becomes especially transparent and elegant for such kind of systems. Section IV gives concluding remarks.

## II. THE AVERAGING METHOD

Consider a tight-binding model with the Hamiltonian

$$H = J \sum (|n\rangle\langle n+1| + |n+1\rangle\langle n|) + \sum_n V(n)|n\rangle\langle n| + edE(\omega t) \sum_n n|n\rangle\langle n|, \quad (1)$$

where  $J$  is the hopping parameter,  $V(n)$  is the external potential (we consider only parabolic potential in this paper,  $V(n) = V\frac{n^2}{2}$ ),  $d$  is the intersite distance,  $E$  is the applied electric field,  $e$  is the charge of the particle. The same model can be realized also with neutral particles, by appropriate shaking of the lattice.

Expanding a quantum state as  $|\psi(t)\rangle = \sum c_n|n\rangle$ , one gets a system of equations

$$i\dot{c}_n = J(c_{n+1} + c_{n-1}) + V(n)c_n + \mathcal{E}(\omega t)nc_n \quad (2)$$

It is convenient to make a transformation  $c_n(t) = x_n(t) \exp\left[-in \int_0^t \mathcal{E}(t')dt'\right]$ , so that equations of motion are

$$i\dot{x}_n = J(x_{n+1}F(t) + x_{n-1}F^*(t)) + V(n)x_n, \quad (3)$$

where  $F(t) = \exp\left[-i \int_0^t \mathcal{E}(t')dt'\right] = F_0 + \sum F_l \exp(-il\omega t)$ ,  $\mathcal{E} = edE$ .

Introducing fast time  $t' = \omega t \equiv t/\epsilon$ , we get, in the matrix form,

$$i\dot{X} = \epsilon H X, \quad (4)$$

where

$$H = J \begin{pmatrix} 0 & F & \cdots & 0 \\ F^* & 0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & F \\ 0 & \cdots & F^* & 0 \end{pmatrix} \equiv J(F\mathcal{U} + F^*\mathcal{B}), \quad (5)$$

where  $\mathcal{U}, \mathcal{B}$  are matrices with unities on the first upper- and lower- codiagonals, correspondingly ( $\mathcal{U}_{mn} = \delta_{m,n+1}, \mathcal{B}_{mn} = \delta_{m,n-1}$ ).

Secondly, consider the case of the chain with periodic boundary conditions, with the Hamiltonian

$$H_p = J \begin{pmatrix} 0 & F & 0 & \cdots & F^* \\ F^* & 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & \ddots & 0 & F \\ F & 0 & \cdots & F^* & 0 \end{pmatrix} \quad (6)$$

Thirdly, in the case of a lattice with additional parabolic potential ( $V(n) = V\frac{n^2}{2}$ ) often employed in applications with ultracold atoms, the Hamiltonian is

$$H_{pp} = J \begin{pmatrix} \frac{N^2V}{2J} & F & 0 & \cdots & 0 \\ F^* & \frac{(N-1)^2V}{2J} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & \ddots & \frac{(N-1)^2V}{2J} & F \\ 0 & 0 & \cdots & F^* & \frac{N^2V}{2J} \end{pmatrix}, \quad (7)$$

where  $V$  is the strength of the parabolic potential, and the lattice has  $(2N+1)$  sites.

In the spirit of the Hamiltonian averaging method in classical mechanics, we are making a unitary transformation  $X = C\tilde{X}$  so that equations for the transformed variables are

$$i\dot{\tilde{X}} = [C^{-1}\epsilon HC - iC^{-1}\dot{C}]\tilde{X}. \quad (8)$$

We are looking for a transformation of the form  $C = \exp[\epsilon K_1 + \epsilon^2 K_2 + \epsilon^3 K_3]$ , where  $K_i$  are skew-Hermitian time-periodic matrices, which would remove time-dependent terms from the Hamiltonian, leaving only time-independent terms.

Generally, we have

$$\begin{aligned} C &\approx I + \epsilon K_1 + \epsilon^2 \left( \frac{1}{2} K_1^2 + K_2 \right) + \epsilon^3 \left( \frac{1}{6} K_1^3 + \frac{1}{2} (K_1 K_2 + K_2 K_1) + K_3 \right), \\ C^\dagger &\approx I - \epsilon K_1 + \epsilon^2 \left( \frac{1}{2} K_1^2 - K_2 \right) + \epsilon^3 \left( -\frac{1}{6} K_1^3 + \frac{1}{2} (K_1 K_2 + K_2 K_1) - K_3 \right), \end{aligned} \quad (9)$$

where  $I$  is the unity matrix.

In the first order, we have

$$i\dot{K}_1 = H(t) - \langle H(t) \rangle \equiv \{H\}, \quad (10)$$

and therefore  $iK_1 = \int (H - \langle H \rangle) dt = \int \{H\} dt$ . We introduce here curly brackets as taking time-periodic part of a time-dependent function:  $\{X\} \equiv X - \langle X(t) \rangle$ , where  $\langle X(t) \rangle \equiv \frac{1}{2\pi} \int_0^{2\pi} X(t') dt'$ .

In the second order,

$$i\dot{K}_2 = \left\{ HK_1 - K_1 H - \frac{i}{2} (\dot{K}_1 K_1 - K_1 \dot{K}_1) \right\}. \quad (11)$$

In the third order, we finally get

$$\epsilon H_{eff} = \epsilon H_1 + \epsilon^2 H_2 + \epsilon^3 H_3, \quad (12)$$

where

$$\begin{aligned} H_1 &= \langle H \rangle \\ H_2 &= \langle HK_1 - K_1 H - \frac{i}{2} (\dot{K}_1 K_1 - K_1 \dot{K}_1) \rangle \\ H_3 &= \langle HK_2 - K_2 H + \frac{1}{2} (HK_1^2 + K_1^2 H) - K_1 HK_1 - \frac{i}{2} (\dot{K}_1 K_2 - K_1 \dot{K}_2 + \dot{K}_2 K_1 - K_2 \dot{K}_1) \\ &\quad - \frac{i}{6} (\dot{K}_1 K_1^2 + K_1^2 \dot{K}_1 - 2K_1 \dot{K}_1 K_1) \rangle \end{aligned} \quad (13)$$

These general formulas can be applied to particular models, as done in the next Section.

One can also write expressions Eq.(13) in a more compact way:

$$\begin{aligned} H_1 &= \langle H \rangle \\ H_2 &= \frac{1}{2} \langle [\{H\}, K_1] \rangle \\ H_3 &= \langle [H, K_2] + \frac{1}{2} [[H, K_1], K_1] - \frac{i}{2} ([\dot{K}_1, K_2] + [\dot{K}_2, K_1]) - \frac{i}{6} [[\dot{K}_1, K_1], K_1] \rangle, \end{aligned} \quad (14)$$

where square brackets denote matrix commutation:  $[A, B] = AB - BA$ .

### III. APPLICATIONS TO PARTICULAR MODELS

For the uniform model with periodic boundary conditions (6), we get a very interesting and important result:  $H_2 = H_3 = 0$ . First- and second-order corrections are completely absent in this case (note that, since the Hamiltonian  $\epsilon H_1$  contains  $\epsilon$ ,  $H_2$  and  $H_3$  define the first and the second-order corrections, correspondingly).

For the uniform model with open boundary conditions (5), we have

$$\begin{aligned}
 K_1 &= -i \int \{H\} dt = J \begin{pmatrix} 0 & L & \cdots & 0 \\ -L^* & 0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & L \\ 0 & \cdots & -L^* & 0 \end{pmatrix} = J(L\mathcal{U} - L^*\mathcal{B}), \quad L \equiv \sum_{l \neq 0} \frac{F_l}{l} \exp(-ilt) \\
 \dot{K}_1 &= -i \{H\} = -iJ \begin{pmatrix} 0 & \tilde{F} & \cdots & 0 \\ \tilde{F}^* & 0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \tilde{F} \\ 0 & \cdots & \tilde{F}^* & 0 \end{pmatrix} = -iJ(\tilde{F}\mathcal{U} + \tilde{F}^*\mathcal{B}), \quad \tilde{F} \equiv \{F\} = \sum_{l \neq 0} F_l \exp(-ilt) \\
 HK_1 - K_1H &= J^2 \begin{pmatrix} -P & 0 & \cdots & 0 \\ 0 & 0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & P \end{pmatrix} \equiv -J^2 P \mathcal{Z}_1, \quad P \equiv LF^* + FL^*, \tag{15}
 \end{aligned}$$

where  $\mathcal{Z}_1$  is a square matrix with 1, -1 in the upper left and the bottom right corners, and zeros elsewhere.

$$\dot{K}_1 K_1 - K_1 \dot{K}_1 = iJ^2 D \mathcal{Z}_1 \quad D \equiv L\tilde{F}^* + \tilde{F}L^* \tag{16}$$

$$K_2 = -iJ^2 \mathcal{Z}_1 T, \quad T \equiv \int \left\{ -P + \frac{D}{2} \right\} dt \equiv \int S dt, \tag{17}$$

$$\dot{K}_2 = -iJ^2 \mathcal{Z}_1 S \tag{18}$$

$$HK_2 - K_2H = iTJ^3 \begin{pmatrix} 0 & F & 0 & \cdots & 0 \\ -F^* & 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & \ddots & 0 & F \\ 0 & 0 & \cdots & -F^* & 0 \end{pmatrix} = iTJ^3(F\mathcal{U}_1 - F^*\mathcal{B}_1), \quad (19)$$

where  $\mathcal{U}_1, \mathcal{B}_1$  are matrices with only two non-zero entries '1' on the ends of the upper- and lower-co-diagonal.

$$\frac{1}{2}(HK_1^2 + K_1^2H) - K_1HK_1 = -\frac{PJ^3}{2}(L\mathcal{U}_1 + L^*\mathcal{B}_1) \quad (20)$$

$$\frac{i}{6}(\dot{K}_1K_1^2 + K_1^2\dot{K}_1 - 2K_1\dot{K}_1K_1) = -\frac{DJ^3}{6}(L\mathcal{U}_1 + L^*\mathcal{B}_1) \quad (21)$$

$$\frac{i}{2}(\dot{K}_1K_2 - K_1\dot{K}_2 + \dot{K}_2K_1 - K_2\dot{K}_1) = \frac{J^3}{2}(S[L\mathcal{U}_1 + L^*\mathcal{B}_1] + iT[\tilde{F}\mathcal{U}_1 - \tilde{F}^*\mathcal{B}_1]). \quad (22)$$

One obtains

$$\langle P \rangle = \langle D \rangle = 2 \sum_{l=1} \frac{|F_l|^2 - |F_{-l}|^2}{l} \equiv 2D_2. \quad (23)$$

$$\langle LD \rangle = \sum_{k \neq 0} \sum_{l \neq 0} \left( \frac{F_k F_l F_{k+l}^* + F_k F_l^* F_{l-k}}{kl} \right) \equiv L_3, \quad (24)$$

$$\langle TF \rangle = \frac{i}{2} L_3. \quad (25)$$

To conclude, in the case of open boundary conditions effective Hamiltonians have a very simple form

$$H_2 = J^2 D_2 \mathcal{Z}_1, \quad H_3 = -\frac{J^3}{3}(L_3 \mathcal{U}_1 + L_3^* \mathcal{B}_1). \quad (26)$$

Thirdly, in the model with parabolic potential (7) we have

$$K_1 = J(L\mathcal{U} - L^*\mathcal{B}), \quad \dot{K}_1 = J(\tilde{F}\mathcal{U} + \tilde{F}^*\mathcal{B}), \quad (27)$$

$$\dot{K}_1 K_1 - K_1 \dot{K}_1 = iJ^2 DZ_1 \quad (28)$$

$$HK_1 - K_1H = J^2 \begin{pmatrix} -P & \frac{2N-1}{2} \frac{V}{J} L & 0 & \cdots & 0 \\ \frac{2N-1}{2} \frac{V}{J} L^* & 0 & \frac{2N-3}{2} \frac{V}{J} L & 0 & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & \ddots & 0 & -\frac{2N-1}{2} \frac{V}{J} L \\ 0 & 0 & \cdots & -\frac{2N-1}{2} \frac{V}{J} L^* & P \end{pmatrix} \quad (29)$$

The first correction to the averaged Hamiltonian  $\epsilon^2 H_2$  looks exactly the same as that of the uniform case, and does not depend on the potential. In the following, we neglect influence of the boundary conditions, assuming the lattice is very long. Then, the first correction is absent, while the second correction  $\epsilon^3 H_3 = \epsilon^3 J^2 V M$  contains contribution from the parabolic potential.  $M$  is a 5-diagonal matrix, with the following entries (non-zero diagonals are listed from top to bottom, with ('0') denoting the main diagonal, ('+2') and ('+1') upper co-diagonals, ('-2') and ('-1') lower co-diagonals) :

$$\begin{aligned} ('+2') & \quad (i\langle FL_2 \rangle - \frac{i}{2}\langle \tilde{F}L_2 \rangle)\delta_{m,n+2} \\ ('+1') & \quad 0 \\ ('0') & \quad (-i\langle F^*L_2 + FL_2^* \rangle + \frac{i}{2}\langle \tilde{F}^*L_2 + \tilde{F}L_2^* \rangle)\delta_{m,n} \\ ('-1') & \quad 0 \\ ('-2') & \quad (i\langle F^*L_2^* \rangle - \frac{i}{2}\langle \tilde{F}^*L_2^* \rangle)\delta_{m,n-2}, \end{aligned} \quad (30)$$

$$L_2 = i \sum_{l \neq 0} \frac{F_l}{l^2} \exp(-ilt), \quad \langle L_2 \rangle = 0, \quad \langle FL_2 \rangle = \langle \tilde{F}L_2 \rangle = i \sum_{l \neq 0} \frac{F_l F_{-l}}{l^2}$$

One can see that this correction creates next-nearest-neighbour couplings: non-zero entries are not on the main co-diagonals, as it would be in case of nearest-neighbour couplings, but on the next-to main co-diagonals. Since  $\langle F^*L_2 + FL_2^* \rangle = \left\langle \left( \sum_{l \neq 0} F_l^* \exp(ilt) i \sum_{m \neq 0} \frac{F_m}{m^2} \exp(-imt) \right) + \right.$

$\left( \sum_{l \neq 0} F_l \exp(-ilt) (-i) \sum_{m \neq 0} \frac{F_m^*}{m^2} \exp(imt) \right) \rangle = 0$ , finally the second correction has a very simple, two-diagonal form

$$\epsilon^3 H_3^{mn} = \epsilon^3 J^2 V \frac{i}{2} (\langle F L_2 \rangle \delta_{m,n+2} + \langle F^* L_2^* \rangle \delta_{m,n-2}) \quad (31)$$

$$= -\frac{\epsilon^3}{2} J^2 V \left( \sum_{l \neq 0} \delta_{m,n+2} \frac{F_l F_{-l}}{l^2} + \delta_{m,n-2} \frac{F_l^* F_{-l}^*}{l^2} \right) \quad (32)$$

Consider a particular case of harmonic driving, with  $\mathcal{E} = \mathcal{E}_0 \cos t$ . We have  $F_l = J_l(\mathcal{E}_0)$ . The induced next-nearest neighbour coupling is  $J' = -\epsilon^3 J^2 V \sum_{l>0} \frac{(-1)^l J_l^2(\mathcal{E}_0)}{l^2}$

Returning from the fast time back to the original time, we have

$$J' = -\frac{J^2 V}{\omega^2} \sum_{l>0} \frac{(-1)^l J_l^2(\mathcal{E}_0)}{l^2} \quad (33)$$

As a function of  $\mathcal{E}_0$ , it has an oscillatory form, and one can choose parameters that nullify the next-neighbour coupling (e.g.,  $\mathcal{E}_0 = 3.32, 4.11$ , etc), or maximize it (e.g.,  $\mathcal{E}_0 = 1.77, 5.24$ , etc). It can be tuned to be either positive or negative, which may be useful for applications.

#### IV. CONCLUSIONS

The approach based on canonical transformations and described in Section II has been applied to three different lattice systems: uniform lattice with open boundary conditions, uniform lattice with periodic boundary conditions, and a lattice with an additional parabolic potential. In the first case, we generalize results obtained by S. Longhi [10]. In particular, we show that second-order corrections have very simple ('boundary') form. In the second case, we get a very interesting and unexpected result: absence of corrections to the averaged Hamiltonian in the second and third order. In the case of external parabolic potential, another unexpected result is found: interplay of driving and non-uniform external potential creates effective (uniform!) next-nearest neighbour couplings. The same result can be obtained in the semiclassical approach [14]. These results, we believe, may find applications in forthcoming experiments with cold atoms in driven optical lattices.

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